

PENALIZED EUCLIDEAN DISTANCE REGRESSION

D. VASILIU, T. DEY, AND I.L. DRYDEN

ABSTRACT. A new method is proposed for variable screening, variable selection and prediction in linear regression problems where the number of predictors can be much larger than the number of observations. The method involves minimizing a penalized Euclidean distance, where the penalty is the geometric mean of the ℓ_1 and ℓ_2 norms of the regression coefficients. This particular formulation exhibits a grouping effect, which is useful for screening out predictors in higher or ultra-high dimensional problems. Also, an important result is a signal recovery theorem, which does not require an estimate of the noise standard deviation. Practical performances of variable selection and prediction are evaluated through simulation studies and the analysis of a dataset of mass spectrometry scans from melanoma patients.

Keywords. Euclidean distance; Grouping; Penalization; Prediction; Regularization; Sparsity; Variable screening.

1. INTRODUCTION

High dimensional regression problems are of great interest in a wide range of applications, for example in analysing microarrays (Hastie et al., 2008; Fan et al., 2009), functional magnetic resonance images (Caballero Gaudes et al., 2013) and mass spectrometry data (Tibshirani et al., 2005). We consider the problem of predicting a single response Y from a set of p predictors X_1, \dots, X_p , where p can be much larger than the number of observations n of each variable. If $p > n$, commonly used methods include regularization by adding a penalty to the least squares objective function or variable selection of the most important predictors.

A wide range of methods is available for achieving one or both of the essential goals in linear regression: accomplishing predictive accuracy and identifying pertinent predictive variables. There is a very large literature on high-dimensional regression methods, for example introductions to the area are given by Hastie et al. (2008) and James et al. (2013). Earlier methods for high-dimensional regression include procedures which minimize a least squares objective function plus a penalty on the regression parameters. The methods include ridge regression (Hoerl and Kennard, 1970a,b) with a squared ℓ_2 penalty; LASSO (Tibshirani, 1996) with an ℓ_1 penalty; and the Elastic Net (Zou and Hastie, 2005) with a linear combination of ℓ_1 and squared ℓ_2 penalties. Alternative methods include the Dantzig selector (Candes and Tao, 2007), where the correlation between the residuals and predictors is bounded; Sure Independence Screening (Fan and Lv, 2008) where predictors are initially screened using componentwise regression; and Square Root LASSO (Belloni et al, 2011), which involves minimizing the square root of the least squares objective function (a Euclidean distance) plus an ℓ_1 penalty. Belloni et al (2011) have given a rationale

for choosing the regularization parameter using a property called pivotal recovery, without requiring an estimate of the noise standard deviation.

We also use a Euclidean distance objective function in our method plus a new norm based on the geometric mean of the ℓ_1 and ℓ_2 norms of the regression parameters. The advantage of our approach is that we are also able to provide the pivotal recovery property, but in addition gain the grouping property of the Elastic Net. The resulting penalized Euclidean distance method is shown to work well in a variety of settings. A particularly strong feature is that it works well when there are correlated designs with weak signal and strong noise.

2. PENALIZED EUCLIDEAN DISTANCE

2.1. Notation. We assume that the data are organized as an $n \times p$ design matrix X , and a n dimensional response vector Y , where n is the number of observations and p is the number of variables. The columns of the matrix X , are $x_{*,j} := (x_{1,j}, x_{2,j}, \dots, x_{n,j})^T$, $j = 1, \dots, p$ and the regression parameters are $\beta = (\beta_1, \dots, \beta_p)^T$. The usual linear model is $Y = X\beta + \sigma\epsilon$ where $E[\epsilon] = 0$ and $\text{var}(\epsilon) = I_n$, and I_n is the $n \times n$ identity matrix. We shall assume that the expectation of the response $Y = (y_1, y_2, \dots, y_n)^T$ depends only on a few variables, and so

$$(1) \quad X\beta = \tilde{X}\tilde{\beta},$$

where the columns of the matrix \tilde{X} are a subset of the set of columns of the entire design matrix X , so \tilde{X} is associated with a subset of indices $\tilde{\mathcal{J}} \subset \{1, 2, \dots, p\}$ and $\tilde{\beta}$ is a vector whose dimension is equal to the cardinality of $\tilde{\mathcal{J}}$. We call the columns in \tilde{X} the “drivers” of the model. We make the observation that in general, $\tilde{\mathcal{J}}$ may not be unique since an underdetermined system could have solutions with different sparsity patterns, even if the degree of the optimal sparsity (model size) is the same. However, in the signal reconstruction problem that we consider, where a penalty on the parameters is introduced, we shall assume that there is a unique solution. The cardinality of $\tilde{\mathcal{J}}$ is assumed to be less than the number of observations and it is desirable that the columns of \tilde{X} are linearly independent. When p is much greater than $|\tilde{\mathcal{J}}|$ a huge challenge is to detect the set of irrelevant columns, i.e. the variables that are not needed for efficiently controlling the response Y .

2.2. PED objective function. Our method involves minimizing the Euclidean distance between Y and $X\beta$, with a penalty based on the geometric mean of the ℓ_1 and ℓ_2 norms. In particular, we minimize

$$(2) \quad L_{PED}(\lambda, \beta) = \|Y - X\beta\| + \lambda \sqrt{\|\beta\| \cdot \|\beta\|_1}$$

where λ is scalar regularization parameter, $\beta = (\beta_1, \beta_2, \dots, \beta_p)$ is a vector in \mathbb{R}^p , $\|\beta\|^2 = \sum_{j=1}^p \beta_j^2$ is the squared ℓ_2 norm and $\|\beta\|_1 = \sum_{j=1}^p |\beta_j|$, the ℓ_1 norm. The penalized Euclidean distance (PED) estimator $\hat{\beta}$ is defined as the

minimizer of the objective function (2), i.e. $\hat{\beta} = (\hat{\beta}_1, \hat{\beta}_2, \dots, \hat{\beta}_p)$ and

$$(3) \quad \hat{\beta}(\lambda) = \arg \min_{\beta \in \mathbb{R}^p} \{L_{PED}(\lambda, \beta)\}.$$

The penalty is proportional the geometric mean of the ℓ_1 and ℓ_2 norms and has only one control parameter, λ . An alternative, well-established method that combines ℓ_1 and ℓ_2 penalties in a linear manner is the Elastic Net (Zou and Hastie, 2005), which is based on the naïve Elastic Net criterion

$$L_{nen}(\lambda_1, \lambda_2, \beta) = \|Y - X\beta\|^2 + \lambda_2 \|\beta\|^2 + \lambda_1 \|\beta\|_1$$

where $\hat{\beta}_{en} = \sqrt{1 + \lambda_2} \hat{\beta}_{nen}$ and $\hat{\beta}_{nen} = \arg \min_{\beta} \{L_{nen}(\lambda_1, \lambda_2, \beta)\}$. The LASSO (Tibshirani, 1996) is a special case with $\lambda_1 > 0, \lambda_2 = 0$ and ridge regression has $\lambda_1 = 0, \lambda_2 > 0$, and so the Elastic Net combines the two methods. Our PED method also combines features of LASSO and Ridge Regression but in a radically different way. The PED penalty is identical to the LASSO penalty for a single non-zero β_i , and so for very sparse models behaviour like the Square Root LASSO is envisaged. We shall show that for PED there is a grouping effect for correlated variables, which is a property shared by the Elastic Net.

2.3. Standardizing to the unit hyper-sphere. By applying a location transformation, both the design matrix X and the response vector Y can be centred, and we also scale the predictors so that

$$(4) \quad \sum_{i=1}^n y_i = 0, \quad \sum_{i=1}^n x_{i,j} = 0, \quad \sum_{i=1}^n x_{i,j}^2 = 1, \quad j = 1, \dots, p.$$

Note that each covariate $x_{*,j}$ can be regarded as a point on the unit hypersphere S^{n-1} with a centring constraint. We assume that the global minimum of $\|Y - \tilde{X}\tilde{\beta}\|$ is very small, but nonetheless positive

$$\min_{\tilde{\beta} \in \mathbb{R}^{|\tilde{\mathcal{J}}|}} \|Y - \tilde{X}\tilde{\beta}\| \geq c > 0,$$

as obtained in the presence of noise and when the number of observations is larger than $|\tilde{\mathcal{J}}|$, and $\tilde{X}, \tilde{\beta}, |\tilde{\mathcal{J}}|$ were defined after (1). Given this situation and since we define the PED objective function through the sparsity of the solution and the minimization of the norm of the residual, we exclude the possibility of exact solutions.

For any vector $\beta \in \mathbb{R}^p$, we denote by θ_j the angle between $x_{*,j}$ and $Y - X\beta$. Thus for a vector $\tilde{\beta}$ that achieves the global minimum of $\|Y - \tilde{X}\tilde{\beta}\|$, we must have $\theta_j = \frac{\pi}{2}$ for $j \in \tilde{\mathcal{J}}$ and we can define the set of solutions as

$$\mathcal{S} = \{\beta \in \mathbb{R}^p \mid \theta_j = \frac{\pi}{2} \forall j \in \tilde{\mathcal{J}} \text{ and } \beta_j = 0 \forall j \in \tilde{\mathcal{J}}^c\}$$

where $\tilde{\mathcal{J}}^c$ denotes the complement of $\tilde{\mathcal{J}}$ in the set of all indexes $\{1, 2, \dots, p\}$. We also assume that \mathcal{S} is bounded away from $0_{\mathbb{R}^p}$ (i.e. $\beta = 0_{\mathbb{R}^p}$ cannot be a solution for minimizing $\|Y - X\beta\|$). Given these minimal and common sense assumptions, our goal is to build an estimator of the index set \mathcal{S} . Also, thinking of covariates as vectors on the unit

hypersphere S^{n-1} , we would like to build an objective function that facilitates automatic detection of “overcrowding”, where we have a group of very close observations on the hypersphere (where the great circle distances are small within the group) which correspond to highly correlated predictors, which in turn will have similar estimated regression parameters. Throughout the paper we assume that Y have been centered and the columns of X have been standardized as described above.

3. THEORETICAL RESULTS

3.1. Geometric mean norm and grouping. The PED objective function will enable variable selection without imposing restrictive conditions on the data. The concept is based on the simple fact that the sum of the squares of the relative sizes of vector components is always equal to 1. For any vector in \mathbb{R}^p , if there are components that have relative size larger than $\frac{1}{\sqrt{p}}$ then the other components must have relative size falling under this value. In addition if many components have similar relative size due to a grouping effect, then the relative size of those components must be small. The new penalty that we consider is actually a non-standard norm.

Lemma 1. *Given any two p -norms $f, g : \mathbb{R}^n \rightarrow [0, +\infty)$, i.e. for some $p_1, p_2 \geq 1$, $f(\beta) = \left(\sum_{i=1}^n |\beta_i|^{p_1} \right)^{\frac{1}{p_1}}$, $g(\beta) = \left(\sum_{i=1}^n |\beta_i|^{p_2} \right)^{\frac{1}{p_2}}$, we have that $\sqrt{f \cdot g}$ is a norm.*

The following two theorems demonstrate the grouping effect achieved by a minimizer of the penalized Euclidean distance.

Theorem 1. *Let $\hat{\beta}(\lambda) = \arg \min_{\beta} \{L_{PED}(\lambda, \beta)\}$. If $x_{*,i} = x_{*,j}$ then $\hat{\beta}_i(\lambda) = \hat{\beta}_j(\lambda)$.*

Considering the situation of very large p compared to n , selecting and grouping variables is an important priority. Theorem 2 below supports the idea of obtaining groups of highly correlated variables, based on the relative size of the corresponding component minimizers of the penalized Euclidean distance objective function.

Theorem 2. *Assume we have a standardized data matrix X , and Y is a centred response vector, as in (4). Let $\hat{\beta}$ be the PED estimate (i.e. $\hat{\beta}(\lambda) = \arg \min_{\beta} \{L_{PED}(\lambda, \beta)\}$ for some $\lambda > 0$). Define*

$$D_{\lambda}(i, j) = \frac{1}{\|\hat{\beta}(\lambda)\|} |\hat{\beta}_i(\lambda) - \hat{\beta}_j(\lambda)|$$

then

$$D_{\lambda}(i, j) \leq \frac{2\sqrt{1 - \rho_{ij}}}{\lambda} \leq \frac{2\theta_{ij}}{\lambda}$$

where ρ_{ij} is the sample correlation i.e. $(x_{*,i})^T(x_{*,j})$, θ_{ij} is the angle between $x_{*,i}$ and $x_{*,j}$, $0 \leq \theta_{ij} \leq \pi/2$.

Note that the grouping property holds for X_j and X_k that are highly (but not perfectly) correlated. This special grouping effect is facilitated by our particular choice for the objective function. Strong overcrowding on the unit hypersphere around an “irrelevant” column would be detected by a dramatic drop in the relative size of the corresponding components of the solution to our objective function.

3.2. Sparsity Properties. It is important and of great interest to consider the case when the number of variables by far exceeds the number of drivers for the optimal sparse model. Therefore the cardinality of the set \mathcal{S} is infinite, and the challenge is to find a sparse solution in it. The starting point of our analysis will be a solution of the penalized Euclidean distance problem defined by (3). As before, we let $\hat{\theta}_j$ represent the angle between vectors X_j and $Y - X\hat{\beta}$. We note that the angle $\hat{\theta}_j$ could be defined as

$$\hat{\theta}_j = \frac{\pi}{2} - \arcsin \left(\frac{x_{*,j}^T (Y - X\hat{\beta})}{\|Y - X\hat{\beta}\|} \right) \quad , \quad 0 \leq \hat{\theta}_j < \pi.$$

whenever $\|Y - X\hat{\beta}\| \neq 0$. Also, let $\hat{k} = \sqrt{\frac{\|\hat{\beta}\|}{\|\hat{\beta}\|_1}}$. It is well known that we have $\frac{1}{\sqrt[p]{p}} \leq \hat{k} \leq 1$ as long as $\hat{\beta} \neq 0_{\mathbb{R}^p}$. Thus a common-sense but not very restrictive assumption would be that $0_{\mathbb{R}^p}$ should not be a minimizer for $\|Y - X\beta\|$.

Lemma 2. *If $\hat{\beta}(\lambda)$ is a solution of (3) then we have that*

$$(5) \quad \frac{\hat{\beta}_j(\lambda)}{\|\hat{\beta}(\lambda)\|} = \hat{k} \left(\frac{2 \cos(\hat{\theta}_j)}{\lambda} - \hat{k} \operatorname{sgn}(\hat{\beta}_j(\lambda)) \right) \quad \text{if } \hat{\beta}_j(\lambda) \neq 0.$$

Proposition 1. *We have*

$$(6) \quad |\cos(\hat{\theta}_j)| \leq \frac{\lambda \hat{k}}{2} \quad \text{if and only if } \hat{\beta}_j(\lambda) = 0.$$

Proposition 2. *If $\hat{\beta}$ is the solution of (3) and its j -th component is nonzero (i.e. $\hat{\beta}_j \neq 0$) then $\operatorname{sgn}(\hat{\beta}_j) = \operatorname{sgn}(X_j^T(Y - X\hat{\beta})) = \operatorname{sgn}(\frac{\pi}{2} - \hat{\theta}_j)$.*

The following two results demonstrate the existence of a minimizing sequence whose terms have the grouping effect property for the relative size of their components.

Lemma 3. *If $\hat{\beta}$ is the solution of (3), we have $\left| \frac{\hat{\beta}_j}{\|\hat{\beta}(\lambda)\|} \right| < M \leq 1$ if and only if $|\cos(\hat{\theta}_j)| \leq \frac{\lambda}{2} \left(\hat{k} + \frac{M}{\hat{k}} \right)$, where M is a constant.*

Proposition 3. *The solution of the penalized Euclidean distance problem (2) given by $\hat{\beta}(\lambda)$, converges to a minimizer of the norm of the residual as the λ approaches 0.*

3.3. Oracle Property. In this section we demonstrate that PED is also able to recover sparse signals without (pre)-estimates of the noise standard deviation or any knowledge about the signal. In Belloni et al (2011) this property is

referred as “pivotal recovery”. An important aspect is that the development of an oracle theorem also brings a solid theoretical justification for the choice of the parameter λ .

Let $Y = X\beta^* + \sigma\epsilon$, where β^* is the true value for β , σ is the standard deviation of the noise and $\epsilon_i, i = 1, \dots, n$, are independent and identically distributed with a law F^* such that $E_{F^*}(\epsilon_i) = 0$ and $E_{F^*}(\epsilon_i^2) = 1$. Let $\tilde{\mathcal{J}} = \text{supp}(\beta^*)$. For any candidate solution $\hat{\beta}$ we can use the notation L for the plain Euclidean loss, i.e. $L(\hat{\beta}) = \|Y - X\hat{\beta}\|$ and the newly introduced norm is denoted by $\|\beta\|_{(1,2)}$, i.e. $\|\beta\|_{(1,2)} = \sqrt{\|\beta\|_1 \|\beta\|}$.

The idea behind the following considerations is the possibility of estimating $\frac{\|X^T \epsilon\|_\infty}{\|\epsilon\|}$ in probability by using the law F^* . Estimation is explained in Belloni et al (2011) as Lemma 1 under the assumptions of Condition 1. We can use the same general result to show that the method we propose is also capable of producing “pivotal” recoveries of sparse signals.

Before stating the main theorem we introduce some more notation and definitions. The solution of the PED objective function is denoted by $\hat{\beta}(\lambda)$. Let $u = \beta^* - \hat{\beta}(\lambda)$, $\|u\|_X = \|Xu\|$, p^* the cardinality of $\tilde{\mathcal{J}}$, $M^* = \|\beta^*\|$, $S = \frac{\|X^T \epsilon\|_\infty}{\|\epsilon\|}$, $c > 1$ and, for brevity, $\bar{c} = \frac{c+1}{c-1}$. Also, we write \tilde{u} for the vector of components of u that correspond to the non-zero β^* elements, i.e. with indices in $\tilde{\mathcal{J}}$. Also, we write \tilde{u}^c for the vector of components of u that correspond to the zero elements of β^* , i.e. with indices in the complement of $\tilde{\mathcal{J}}$. Consider

$$(7) \quad \Delta_{\bar{c}}^* = \left\{ u \in \mathbb{R}^p : u \neq \{0_{\mathbb{R}^p}\}, \|\tilde{u}^c\|_1 \leq \bar{c}\|\tilde{u}\|_1 + \frac{c\sqrt[4]{p}}{c-1} \sqrt[4]{p^* M^*} \right\}.$$

Assume that

$$\bar{k}_{\bar{c}}^* = \min_{u \in \Delta_{\bar{c}}^*} \frac{1}{\sqrt{n}} \frac{\|u\|_X}{\|u\|}.$$

and

$$k_{\bar{c}}^* = \left(1 - \frac{1}{c}\right) \min_{u \in \Delta_{\bar{c}}^*} \frac{\sqrt{p^*} \|u\|_X}{2\|\tilde{u}\|_1 + \sqrt[4]{p} \sqrt[4]{p^* M^*}}$$

are bounded away from 0. We can investigate when these compatibility conditions might hold. Let $\|u\|_X = O(\sqrt{n})$, $\|\tilde{u}\| = O(p^*)$ and so

$$k_{\bar{c}}^* = \sqrt{p^*} O(\sqrt{n}) / (O(p^*) + \sqrt[4]{p} \sqrt[4]{p^* M^*}) = O(\sqrt{n}) / (O(\sqrt{p^*}) + \sqrt[4]{p} \sqrt[4]{p^*} (M^* / \sqrt{p^*})).$$

and $M^* / \sqrt{p^*}$ is bounded. Such compatibility conditions could be easily achieved in the case when $p = n^{1+\alpha_1}$ and $p^* = n^{\alpha_2}$ with $\alpha_1, \alpha_2 > 0$ and $\alpha_1 + \alpha_2 \leq 1$. We also present later a result with certain compatibility conditions for the case when $p > n^2$.

We refer to k_c^* and \bar{k}_c^* as restricted eigenvalues. The terminology is similar to Bickel et al. (2009), although our definition and usage are different here. As stated before, our oracle theorem is based on estimation of $\frac{\|X^T \epsilon\|_\infty}{\|\epsilon\|}$. In the case when the law $F^* = \Phi_0$ is normal, directly following from Lemma 1 of Belloni et al (2011), we have:

Lemma 4. *Given $0 < \alpha < 1$ and some constant $c > 1$, the choice of parametrization $\lambda = \frac{c \sqrt[4]{p}}{\sqrt{n}} \Phi_0^{-1} \left(1 - \frac{\alpha}{2p}\right)$ satisfies $\lambda \geq c \sqrt[4]{p} S$ with probability $1 - \alpha$.*

Now we are ready to state the main result:

Theorem 3. (Signal Recovery) *Assume that $\lambda \leq \frac{\rho \sqrt[4]{p} k_c^*}{\sqrt{p^*}}$ for some $0 < \rho < 1$. If also $\lambda \geq c \sqrt[4]{p} S$ then we have*

$$(8) \quad (1 - \rho^2) \|u\|_X \leq \frac{2c \sqrt{p^* \log(2p/\alpha)} L(\beta^*)}{k_c^* \sqrt{n}}.$$

A direct consequence is the following oracle inequality:

$$\bar{k}_c^* \|\hat{\beta}(\lambda) - \beta^*\| \leq \frac{\text{const.} \sqrt{p^* \log(2p/\alpha)} L(\beta^*)}{(1 - \rho^2)n},$$

and hence if $L(\beta^*) = O_p(\sqrt{n})$ and $n \rightarrow \infty$ such that $\sqrt{p^* \log(2p/\alpha)}/\sqrt{n} \rightarrow 0$, then we have $\hat{\beta}(\lambda) \rightarrow \beta^*$ in probability.

We can use the value of λ in Lemma 4 for practical implementation in order to ensure $\lambda \geq c \sqrt[4]{p} S$ holds with probability $1 - \alpha$. Note that the rate of convergence is asymptotically the same as rates seen in other sparse regression problems (e.g. see Negahban et al., 2012), although as for the square root LASSO of Belloni et al. (2011) knowledge of σ is not needed. Also there are some circumstances when we can consider other values of λ , as shown in the Corollary.

Corollary 1. *Let $0 < \xi < 1$ and*

$$\Delta_\xi = \left\{ u \in \mathbb{R}^p, \frac{\sqrt{n}}{\sqrt[4]{p}} \|\tilde{u}^c\|_1 \xi \leq \|\tilde{u}\|_1 \left(\frac{2\sqrt{n}}{\sqrt[4]{p}} - \xi \right) + \|\beta^*\|_1 \left(1 - \frac{\sqrt{n}}{\sqrt[4]{p}} \right) \right\}.$$

If $k_\xi^* = \min_{u \in \Delta_\xi} \frac{\frac{\sqrt{p^*}}{\sqrt{n}} \|u\|_X}{\xi \frac{2\sqrt{n}}{\sqrt[4]{p}} \|\tilde{u}\|_1 + \frac{\|\beta^*\|_1}{\xi} \left(1 - \frac{\sqrt{n}}{\sqrt[4]{p}}\right)} > k > 0$ and for $\lambda = c \Phi_0^{-1} \left(1 - \frac{\alpha}{2p}\right) \frac{\sqrt[4]{p}}{n}$, with $c > 1$, we can check $\sqrt{\frac{\|\hat{\beta}(\lambda)\|}{\|\hat{\beta}(\lambda)\|_1}} - \frac{\sqrt{n}}{c \sqrt[4]{p}} \geq \xi > 0$ and, at the same time, we assume $\lambda \leq \frac{\rho \sqrt[4]{p} k_\xi^*}{\sqrt{n} \sqrt{p^*}}$ for some $0 < \rho < 1$ then we also have an oracle property, i.e.

$$\|\hat{\beta}(\lambda) - \beta^*\| \leq \text{const.} \sqrt{\frac{p^* \log(2p/\alpha)}{n}}$$

with probability $1 - \alpha$.

We use the corollary to suggest a method for choosing the model parameters by maximizing

$$(9) \quad \hat{k} = \sqrt{\frac{\|\hat{\beta}(\lambda)\|}{\|\hat{\beta}(\lambda)\|_1}}.$$

Although the compatibility conditions require $p \leq n^2$ if we assume that $\min_{u \in \Delta_\xi} \frac{1}{\sqrt{n}} \frac{\|u\|_X}{\|u\|_1}$ is bounded away from 0, we could allow $p > n^2$ and a sufficient condition for the compatibility inequality invoked by the Corollary would be to have $\sqrt{\frac{\|\hat{\beta}(\lambda)\|}{\|\hat{\beta}(\lambda)\|_1}} > \xi > 0$ for all n . Such a condition is not unrealistic if the set of columns of the design matrix X has a finite partition by subsets of highly correlated covariates. If we have that the set of all indices has always a finite partition by subsets of indices whose corresponding columns in the design matrix X maintain strong correlations. Thus we assume

$$\{1, 2, 3, \dots, p\} = \bigcup_{k=1}^m \mathfrak{J}_k$$

where $m < \infty$ when $n \rightarrow \infty$. If for each subset \mathfrak{J}_k the columns of X whose indices are in \mathfrak{J}_k have the lowest pairwise correlation, ρ_k , such that

$$1 - \rho_k = O\left(\frac{\sqrt{p}}{n^2 |\mathfrak{J}_k|^2}\right)$$

then, based on Theorem 2, we can show that $\frac{\|\hat{\beta}(\lambda)\|_1}{\|\hat{\beta}(\lambda)\|}$ is bounded when $n \rightarrow \infty$ and implicitly the compatibility condition from the Corollary is satisfied.

For a practical implementation of our method we exclusively use the proven theoretical results. From the signal recovery theorem and corollary we obtain that $\|\hat{\beta}(\lambda) - \beta^*\| \leq \text{const.} \sqrt{p^* \log(2p/\alpha)} / \sqrt{n}$ with probability $1 - \alpha$. Thus, if j is an index where there is no signal, i.e. $\beta_j^* = 0$ then, from the previous inequality, we have that $|\hat{\beta}_j(\lambda)| < \|\hat{\beta}(\lambda) - \beta^*\| \leq \text{const.} \sqrt{p^* \log(2p/\alpha)} / \sqrt{n}$. If $\|\hat{\beta}(\lambda)\| \neq 0$ we can divide the constant by $\|\hat{\beta}(\lambda)\|$ and get

$$(10) \quad \frac{|\hat{\beta}_j(\lambda)|}{\|\hat{\beta}(\lambda)\|} < C(p) / \sqrt{n},$$

where

$$(11) \quad C(p) \propto \sqrt{p^* \log(2p/\alpha)}.$$

We will use (10) to inform a threshold choice as part of the PED fitting algorithm. As well as dependence on n we also investigate the effect of p on the relative size of the components. Note that the components of $\hat{\beta}(\lambda)$ whose relative size (i.e. $\frac{|\hat{\beta}_j(\lambda)|}{\|\hat{\beta}(\lambda)\|}$) is small belong to columns of X that make with $Y - X\hat{\beta}(\lambda)$ an angle a lot closer to $\frac{\pi}{2}$ than the rest of the columns. For example, since $1/\sqrt[4]{p} \leq \hat{k} \leq 1$ and if $\frac{|\hat{\beta}_j(\lambda)|}{\|\hat{\beta}(\lambda)\|} < \frac{C(p)}{\sqrt{n}}$ for some $C(p) > 0$, from equation

(5) we have

$$(12) \quad \cos(\hat{\theta}_j) < \frac{\lambda}{2} \left(\hat{k} + \frac{C(p)}{\hat{k}\sqrt{n}} \right) \leq \frac{\lambda}{2} \left(\hat{k} + \frac{C(p)p^{1/4}}{n^{1/2}} \right),$$

and remember $\lambda = O(\sqrt[4]{p}/\sqrt{n})$.

For a practical method we implement the detection of a set $I(\lambda, \delta)$ of “irrelevant” indices (with zero parameter estimates) as follows

$$(13) \quad I(\lambda, C(p)) = \left\{ j, \frac{|\hat{\beta}_j(\lambda)|}{\|\hat{\beta}(\lambda)\|} < \frac{C(p)}{\sqrt{n}} \right\},$$

where $C(p)$ is a threshold value defined in (11) that needs to be chosen. We construct a new vector $\hat{\hat{\beta}}(\lambda)$ which satisfies $\hat{\hat{\beta}}_j(\lambda) = 0$, if $j \in I(\lambda, C(p))$ and the rest of the components give a minimizer of

$$\|Y - \hat{X}\hat{\beta}\| + \lambda\sqrt{\|\hat{\beta}\| \cdot \|\hat{\beta}\|_1}$$

where \hat{X} is obtained from X by dropping the columns with indices in $I(\lambda, C(p))$.

In the next section we show how these results can be implemented in an algorithm for finding sparse minimizers of $L(\beta)$.

4. THE PED ALGORITHM

The objective function $L_{PED}(\lambda, \beta) = \|Y - X\beta\| + \lambda\sqrt{\|\beta\| \cdot \|\beta\|_1}$ is convex for any choice of λ and also differentiable on all open orthants in \mathbb{R}^p bounded away from the hyperplane $Y - X\beta = 0$. In order to find good approximations for minimizers of our objective function, as in many cases of nonlinear large scale convex optimization problems, a Quasi-Newton method may be strongly favoured. A Quasi-Newton method would be preferred since it is known to be considerably faster than methods like coordinate descent by achieving super-linear convergence rates. Another important advantage is that second-derivatives (Hessians) are not necessarily required. For testing purposes, we present an algorithm based on the well performing Quasi-Newton methods for convex optimization known as Broyden-Fletcher-Goldfarb-Shanno (BFGS) methods: limited-memory BFGS (Nocedal, 1980) and BFGS (Bonnans *et al*, 2006). We also tested a version of non-smooth BFGS called Hybrid Algorithm for Non-Smooth Optimization (HANSO) (Lewis and Overton, 2008) and obtained very similar results.

The PED algorithm is:

- (1) Implement the L-BFGS algorithm to minimize the objective function (2) using $\lambda = \lambda_0$.
- (2) Set $\hat{\beta}_j = 0$ if $\frac{|\hat{\beta}_j|}{\|\hat{\beta}\|} \leq C(p)/\sqrt{n}$ (the choice of $C(p)$ is motivated by (12)). Eliminate the columns of the design matrix corresponding to the zero coefficients $\hat{\beta}_j$, with p_0^* non-zero columns remaining.
- (3) (optional) For i in 1 to N :
 - { Use the L-BFGS algorithm to minimize the objective function with $\lambda = \lambda_i < \lambda_{i-1}$.

Set $\hat{\beta}_j = 0$ if $\frac{|\hat{\beta}_j|}{\|\hat{\beta}\|} \leq \frac{C(p_{i-1}^*)}{\sqrt{n}}$. Eliminate the columns of the design matrix corresponding to the zero coefficients $\hat{\beta}_j$, with p_i^* non-zero columns remaining.}

(4) Use the L-BFGS algorithm to minimize the objective function with small λ_F with p adapted to p^* .

The algorithm uses the theoretically informed parameters $\lambda_i, i = 0, \dots, N$ (based on Corollary 1), and the threshold parameters $C(p)$. The steps $i = 0, \dots, N$ involve screening unnecessary variables using the irrelevant information criterion and the final step with small λ_F improves the prediction.

We consider a particular version of the algorithm in our examples using choosing λ_0 and $C(p)$ from a grid of values $\lambda \in \{0.2, 0.5, 1\}$ and $C(p) \in \{0.75, 1, 1.25, 1.5\}$ in order to maximize \hat{k} , and of course other grid choices could be used. In addition we do not use step 3 and finally λ_F is based on Theorem 3 with adapted $p = p^*$. The algorithm is a one-pass method. Other possibilities include using Akaike's Information Criterion (AIC) and 10-fold cross-validation to select the parameters.

5. APPLICATIONS

5.1. Simulation study. *Example 1.* We consider a simulation study to illustrate the performance of our method and the grouping effect in the case when $p \geq n$. In this example we compare the results with the Square Root of Lasso method (Belloni et al, 2011) that uses a scaled Euclidean distance as a loss function plus an ℓ_1 penalty term. We also compare the results with both LASSO and Elastic Net methods as they are implemented in the publicly available packages for R. In particular we used 10-fold cross-validation to choose the roughness penalty for LASSO and the Elastic Net using the command `cv.glmnet` in the R package `glmnet` and we use the command `slim` in the R package `flare` with penalty term $\lambda = 1.1\Phi^{-1}(1 - 0.05/(2p))/\sqrt{n}$. We use the one-pass PED algorithm with parameters chosen from a grid to maximize (9). We consider situations with weak signal, strong noise and various correlated designs. In particular, for a range of values of n, p, ρ the data are generated from the linear model $Y = X\beta^* + \sigma\epsilon$, where

$$\beta^* = (\underbrace{0.3, \dots, 0.3}_4, \underbrace{0, \dots, 0}_{50}, \underbrace{0.3, \dots, 0.3}_4, \underbrace{0, \dots, 0}_{50}, \underbrace{0.3, \dots, 0.3}_4, \underbrace{0, \dots, 0}_{50}, \underbrace{0.3, \dots, 0.3}_4, 0, \dots, 0),$$

$\|\beta^*\|_0 = 12$, $\sigma = 1.5$ and X generated from a p -dimensional multivariate normal distribution with mean zero and correlation matrix Σ where the (j, k) -th entry of Σ is $\rho^{|j-k|}$, $1 \leq j, k \leq p$.

The results are summarized in the following table and the reported values are based on averaging over 100 data sets. The distance between the true signal and the solution produced is also recorded. Under highly correlated designs, the method we propose shows a very efficient performance against the ‘‘curse of dimensionality’’ and overcrowding. PED has performed very well, obtaining the highest rate of true positives in many examples. We use the one-pass PED method where the choice of λ_0 is taken such that \hat{k} is an approximate maximum. Also, we compare with PED when the parameters are selected by AIC, given by PED(AIC). The Elastic Net is the next best, and Lasso and

	$\rho = 0.5$			$\rho = 0.9$			$\rho = 0.99$		
	TP	MS	RMSE	TP	MS	RMSE	TP	MS	RMSE
$n = 100, p = 200$									
PED	10.5	28.06	0.933	11.5	27.3	0.742	10.39	41.71	0.879
PED(AIC)	8.19	48.2	1.529	10.2	31.92	1.083	9.26	49.62	0.983
Elastic Net	9.34	30.17	0.949	9.43	25.63	1.064	6.2	23.52	1.436
Lasso	8.75	26.18	0.879	7.38	20.15	1.069	3.59	14.34	1.637
Sq.Rt.Lasso	1.18	1.2	1.015	3.94	4.65	0.927	3.03	8.84	1.291
$n = 100, p = 1000$									
PED	8.79	48.22	1.251	10.91	35.59	0.900	11.14	72.19	0.847
PED(AIC)	8.79	48.11	1.252	10.47	41.7	1.214	9.27	58.15	1.093
Elastic Net	7.93	44.48	1.042	9.46	37.73	1.077	7.51	34.46	1.265
Lasso	7.07	32.27	0.956	6.87	27	1.044	3.3	18.03	1.510
Sq.Rt.Lasso	0.9	0.94	1.025	2.91	3.42	0.965	2.97	9.07	1.253
$n = 200, p = 200$									
PED	11.52	18.64	0.580	11.95	29.08	0.613	11.91	54.95	0.759
PED(AIC)	11.61	49.66	1.019	11.65	25.13	0.721	10.38	34.06	0.823
Elastic Net	11.41	34.3	0.687	10.45	25.57	0.860	7.72	23.53	1.1175
Lasso	11.03	30.89	0.653	8.85	21.59	0.900	5.04	15.3	1.396
Sq.Rt.Lasso	5.42	5.47	0.900	7.26	8.3	0.830	4.84	11.32	1.190
$n = 200, p = 2000$									
PED	11.35	87.89	1.194	9.39	31	0.759	12	114.99	0.763
PED(AIC)	11.35	87.76	1.194	11.84	78.17	1.258	9.94	39.93	0.972
Elastic Net	10.52	57.22	0.794	10.79	42.47	0.835	9.55	37.03	1.007
Lasso	9.79	44.42	0.752	8.65	31.19	0.856	4.77	19.74	1.280
Sq.Rt.Lasso	3.57	3.57	0.961	6.45	7.09	0.837	4.8	11.14	1.155
$n = 200, p = 3000$									
PED	11.21	76.61	1.145	10.18	33.08	0.758	12	121.2	0.763
PED(AIC)	11.21	76.61	1.144	12	59.24	1.053	9.44	46.02	1.067
Elastic Net	10.23	64.83	0.834	10.75	44.16	0.839	9.94	37.42	0.993
Lasso	9.61	49.97	0.788	8.48	33.77	0.870	4.62	19.04	1.293
Sq.Rt.Lasso	2.86	2.87	0.980	6.31	7.05	0.843	4.6	10.79	1.173

TABLE 1. Simulation results based on Example 1. The best values in the TP and RMSE columns are in bold. The True Positives (TP) are the average number of non-zero parameters which are estimated as non-zero and the Model Size (MS) is the average number estimated non-zero parameters, from 100 simulations. The RMSE is given for the $\hat{\beta}$ parameters.

Square root Lasso have low rates of True Positives. PED has a lower model size compared to the Elastic Net. Finally the RMSE is generally best for PED, particularly for the higher correlated situations. Overall PED has performed extremely well in these simulations.

5.2. Mass spectrometry data from melanoma patients. We consider an application of the method to a proteomics dataset from the study of melanoma (skin cancer). The mass spectrometry dataset was described by Mian et al. (2005) and further analysed by Browne et al. (2010). The data consist of mass spectrometry scans from serum samples of 205 patients, with 101 patients with Stage I melanoma (least severe) and 104 patients with Stage IV

melanoma (most severe). Each mass spectrometry scan consists of an intensity for 13951 mass over charge (m/z) values between 2000 and 30000 Daltons. It is of interest to find which m/z values could be associated with the stage of the disease, which could point to potential proteins for use as biomarkers. We first fit a set of 500 important peaks to the overall mean of the scans using the deterministic peak finding algorithm of Browne et al. (2010) to obtain 500 m/z values at peak locations. We consider the disease stage to be the response, with $Y = -1$ for Stage I and $Y = 1$ for Stage IV. Note that we have an ordered response here as Stage IV is much more severe than Stage I, and it is reasonable to treat the problem as a regression problem.

We fit the PED regression model versus the intensities at the 500 peak locations. We have $n = 205$ by $p = 500$. The data are available at <http://www.maths.nottingham.ac.uk/~ild/mass-spec>

Here we consider the one pass PED method, with $\alpha = 0.05$. The parameter values chosen to maximize \hat{k} are $\lambda = 0.5$ and $C(p) = 0.75$, selecting 96 non-zero m/z values. Browne et al. (2010) also considered a mixed effects Gaussian mixture model and a two stage t-test for detecting significant peaks. If we restrict ourselves to the coefficients corresponding to the 50 largest peaks, Browne et al. (2010) identified 17 as non-zero as did PED, with 8 out of the 17 in common. If we apply PED(AIC) then 7 peaks are chosen out of the largest 50 of which only 2 are in common with Browne et al. (2010). The Elastic Net chose 6 peaks with 5 of those in common with Brown et al. (2010) and for the Lasso 5 peaks were chosen from the top 50 largest, with 4 in common with Browne et al. (2010). Note that here PED has selected the most peaks in common with Browne et al. (2010), and it is reassuring that the different methods have selected some common peaks.

6. CONCLUSIONS

We have introduced a sparse linear regression method which does not make use of existing sparse regression algorithms. Backed up by a concrete and relatively simple theoretical explanation, we show that the proposed methodology is useful and practical to implement without imposing any assumptions that in general could be infeasible to verify. A notable aspect is that under correlated designs we did not assume any restrictive conditions between the number of observations and the number of predictors, and so the proposed method has wide range of applicability. Further extensions of the work will follow in a natural way, for example as Fan et al. (2009) have extended ISIS to generalized linear models and classification problems. It will be interesting to analyse the mass spectrometry data using PED for binary response models, and compare this with the PED regression approach of our paper.

The performance of the proposed method has been compared with a number of well known variable selection methods and has performed favourably. Further, the predictive performance of the proposed method has been compared to some current state-of-the-art known predictive techniques and it seems very effective in higher dimensional situations. In conclusion, the method appears to be a promising addition to the sparse regression toolbox.

ACKNOWLEDGEMENT

We would like to thank the editor and the referees for their valuable comments and insight that significantly helped to improve the quality of this manuscript.

REFERENCES

- Belloni, A., Chernozhukov, V., Wang, L. (2011). Square-root lasso: pivotal recovery of sparse signals via conic programming. *Biometrika*, 98, 4, 791 – 806.
- Bickel, P.J., Ritov, Y. and Tsybakov, A. B. (2009). Simultaneous analysis of lasso and Dantzig selector. *Ann. Statist.* 37, 4, 1705–1732.
- Bonnans, J.F., Gilbert, J.C., Lemaréchal, C. and Sagastizábal, C.A. (2006). *Numerical optimization: Theoretical and practical aspects*, Berlin: Springer-Verlag.
- Browne, W.J., Dryden, I.L., Handley, K., Mian, S. and Schadendorf, D. (2010). Mixed effect modelling of proteomic mass spectrometry data using Gaussian mixtures. *Journal of the Royal Statistical Society, Series C (Applied Statistics)*, 59, 617-633.
- Caballero Gaudes, C., Petridou, N., Francis, S., Dryden, I.L. and Gowland, P. (2013). Paradigm Free Mapping with sparse regression automatically detects single-trial fMRI BOLD responses. *Human Brain Mapping*. 34, 501-518.
- Candès, E. and Tao, T. (2007). The Dantzig selector: Statistical estimation when p is much larger than n . *Annals of Statistics*, 35(6), 2313 - 2351.
- Fan, J. and Lv, J. (2008). Sure independence screening for ultra-high dimensional feature space. *Journal of Royal Statistical Society Series B*, 70, 849 - 911.
- Fan, J., Samworth, R. and Wu, Y. (2009). Ultra-high Dimensional Feature Selection: Beyond The Linear Model. *Journal of Machine Learning Research* 10, 2013–2038.
- Hastie, T., Tibshirani, R. and Friedman, J. (2008). *The Elements of Statistical Learning (2nd edition)*, Springer, New York.
- Hoerl A.E. and Kennard R.W. (1970a). Ridge regression: Biased estimation for nonorthogonal problems. *Technometrics*, 12, 55 - 67.
- Hoerl A.E. and Kennard R.W. (1970b). Ridge regression: Applications to nonorthogonal problems (Corr: V12 p723). *Technometrics*, 12, 69 - 82.
- James, G., Witten, D., Hastie, T. and Tibshirani, R. (2013). *An Introduction to Statistical Learning with Applications in R*. Springer, New York.
- Lewis A. S. and Overton, M. L. (2008). Nonsmooth optimization via BFGS. Technical Report, New York University.
- Mian, S., Ugurel, S., Parkinson, E., Schlenzka, I., Dryden, I.L., Lancashire, L., Ball, G., Creaser, C., Rees R., and Schadendorf, D. (2005). Serum proteomic fingerprinting discriminates between clinical stages and predicts

- disease progression in melanoma patients. *Journal of Clinical Oncology*, 33, 5088-5093.
- Negahban, S. N., Ravikumar, P., Wainwright, M. J. and Yu, B. (2012). A unified framework for high-dimensional analysis of M -estimators with decomposable regularizers. *Statist. Sci.*, 27, 538–557.
- Nocedal, J. (1980). Updating Quasi-Newton Matrices with Limited Storage. *Mathematics of Computation*, 35 (151): 773- 782.
- Tibshirani, R. (1996) Regression Shrinkage and Selection via the Lasso. *Journal of the Royal Statistical Society Series B*, 58, 267 – 288.
- Tibshirani, R., Saunders, M., Rosset, S., Zhu, J. and Knight, K. (2005). Sparsity and smoothness via the fused lasso. *J. R. Statist. Soc. B*, 67, pp. 91–108.
- Zou, H. and Hastie, T. (2005). Regularization and variable selection via the Elastic Net. *Journal of the Royal Statistical Society, Series B*, 67, 301 - 320.

APPENDIX A: PROOFS

Proof. (Lemma 1.) Let

$$\mathcal{C} = \{\beta \in \mathbb{R}^n | \sqrt{f(\beta)g(\beta)} \leq 1\}.$$

We notice that $\mathcal{C} \equiv \{\beta \in \mathbb{R}^n | [f(\beta)g(\beta)]^{2p_1 p_2} \leq 1\}$ and therefore \mathcal{C} is a bounded, closed and convex subset of \mathbb{R}^n which contains the origin. Let $\text{Epi}(h)$ denote the epigraph of some function $h : \mathbb{R}^p \rightarrow \mathbb{R}$ i.e. $\text{Epi}(h) = \{(\beta, t) \in \mathbb{R}^{n+1} | h(\beta) \leq t\}$.

We see that in our case $\text{Epi}(\sqrt{f \cdot g}) = \{t(\mathcal{C}, 1) | t \in [0, +\infty)\}$ and therefore $\text{Epi}(\sqrt{f \cdot g})$ is a convex cone in \mathbb{R}^{n+1} since \mathcal{C} is a convex set in \mathbb{R}^n . This shows that $\sqrt{f \cdot g}$ is a convex function. Because $\sqrt{f \cdot g}$ is convex and homogeneous of degree 1 it follows that it must also satisfy the triangle inequality. Therefore $\sqrt{f \cdot g}$ is a norm on \mathbb{R}^n . What we present is the fact that the geometric mean of two p -norms is also a norm on a finite dimensional vector space. \square

Proof. (Theorem 1.) We follow a similar idea as stated in Zou and Hastie (2005). Let $\hat{\beta} = \arg \min_{\beta} \{L_{PED}(\lambda, \beta)\}$ and assume that $x_{*,i} = x_{*,j}$. Let $J(\beta) = \lambda \sqrt{\|\beta\| \|\beta\|_1}$. If $\hat{\beta}_i \neq \hat{\beta}_j$ consider

$$\hat{\beta}_k^* = \begin{cases} \hat{\beta}_k & \text{if } k \neq i \text{ and } k \neq j \\ \frac{1}{2}(\hat{\beta}_i + \hat{\beta}_j) & \text{if } k = i \text{ or } k = j \end{cases}$$

We have $\|Y - X\hat{\beta}\|^2 = \|Y - X\hat{\beta}^*\|^2$. We also consider $J(\hat{\beta}) = \lambda \sqrt{\sum_{k=1}^p |\hat{\beta}_k|} \sqrt{\sum_{k=1}^p \hat{\beta}_k^2}$ and notice that

$$J(\hat{\beta}^*) = \lambda \sqrt{\left(\sum_{\substack{k=1 \\ k \neq i,j}}^p |\hat{\beta}_k| + \frac{1}{2} |\hat{\beta}_i + \hat{\beta}_j| \right)} \sqrt{\sum_{\substack{k=1 \\ k \neq i,j}}^p \hat{\beta}_k^2 + \frac{1}{4} |\hat{\beta}_i + \hat{\beta}_j|^2}$$

It is clear that

$$\left(\sum_{\substack{k=1 \\ k \neq i,j}}^p |\hat{\beta}_k| + \frac{1}{2} |\hat{\beta}_i + \hat{\beta}_j| \right) \sqrt{\sum_{\substack{k=1 \\ k \neq i,j}}^p \hat{\beta}_k^2 + \frac{1}{4} |\hat{\beta}_i + \hat{\beta}_j|^2} < \left(\sum_{k=1}^p |\hat{\beta}_k| \right) \sqrt{\sum_{k=1}^p \hat{\beta}_k^2}$$

which implies $J(\hat{\beta}^*) < J(\hat{\beta})$, a contradiction with the fact that $\hat{\beta} = \arg \min_{\beta} \{L_{PED}(\lambda, \beta)\}$. \square

Proof. (Theorem 2.) If $x_{*,i} = x_{*,j}$ then $\hat{\beta}_i = \hat{\beta}_j$ which means that the proposed regression method should assign identical coefficients to the identical variables. Since $\hat{\beta}(\lambda) = \arg \min_{\beta} \{L_{PED}(\lambda, \beta)\}$ we have

$$(14) \quad \left. \frac{\partial L_{PED}(\lambda, \beta)}{\partial \beta_k} \right|_{\beta=\hat{\beta}(\lambda)} = 0 \text{ for every } k = 1, 2, \dots, p$$

unless $\hat{\beta}_k(\lambda) = 0$. Thus, if $\hat{\beta}_k(\lambda) \neq 0$ we have

$$(15) \quad -\frac{x_{*,k}^T [Y - X\hat{\beta}(\lambda)]}{\|Y - X\hat{\beta}(\lambda)\|} + \frac{\lambda}{2} \frac{\frac{\hat{\beta}_k(\lambda)}{\|\hat{\beta}(\lambda)\|} |\hat{\beta}(\lambda)|_1}{\sqrt{\|\hat{\beta}(\lambda)\| \cdot |\hat{\beta}(\lambda)|_1}} + \frac{\lambda \operatorname{sgn}\{\hat{\beta}_k(\lambda)\} \|\hat{\beta}(\lambda)\|}{2 \sqrt{\|\hat{\beta}(\lambda)\| \cdot |\hat{\beta}(\lambda)|_1}} = 0.$$

If we take $k = i$ and $k = j$, after subtraction we obtain

$$(16) \quad \frac{[x_{*,j}^T - x_{*,i}^T][Y - X\hat{\beta}(\lambda)]}{\|Y - X\hat{\beta}(\lambda)\|} + \frac{\lambda}{2} \frac{[\hat{\beta}_i(\lambda) - \hat{\beta}_j(\lambda)] |\hat{\beta}(\lambda)|_1}{\sqrt{\|\hat{\beta}(\lambda)\|^3 \cdot |\hat{\beta}(\lambda)|_1}} = 0$$

since $\operatorname{sgn}\{\hat{\beta}_i(\lambda)\} = \operatorname{sgn}\{\hat{\beta}_j(\lambda)\}$. Thus we get

$$(17) \quad \frac{\hat{\beta}_i(\lambda) - \hat{\beta}_j(\lambda)}{\|\hat{\beta}(\lambda)\|} = \frac{2}{\lambda} \frac{\sqrt{\|\hat{\beta}(\lambda)\| \cdot |\hat{\beta}(\lambda)|_1}}{|\hat{\beta}(\lambda)|_1} [x_{*,j}^T - x_{*,i}^T] \hat{r}(\lambda)$$

where $\hat{r}(\lambda) = \frac{y - X\hat{\beta}(\lambda)}{\|y - X\hat{\beta}(\lambda)\|}$ and $\|x_{*,j}^T - x_{*,i}^T\|^2 = 2(1 - \rho)$ since X is standardized, and $\rho = \cos(\theta_{ij})$. We have $\frac{\sqrt{\|\beta\| \cdot \|\beta\|_1}}{\|\beta\|_1} \leq 1$ for any nonzero vector β in \mathbb{R}^p and $|\hat{r}(\lambda)| \leq 1$. Thus, equation (17) implies that

$$(18) \quad D_\lambda(i, j) \leq \frac{2|\hat{r}(\lambda)|}{\lambda} \|x_{*,i} - x_{*,j}\| \leq \frac{2}{\lambda} \sqrt{2(1 - \rho)} < 2 \frac{\theta_{ij}}{\lambda},$$

which proves the grouping effect property for the proposed method. \square

Proof. (Proposition 1) Here we are going to prove the “if” part as the “only if” implication follows directly from the previous Lemma. Let us assume that

$$\hat{\beta}(\lambda) = (\hat{\beta}_1(\lambda), \dots, \hat{\beta}_{j-1}(\lambda), 0, \hat{\beta}_{j+1}(\lambda) \dots \hat{\beta}_p(\lambda)) = \arg \min_{\beta} \{L_{PED}(\lambda, \beta)\}$$

for a given $\lambda > 0$. Here we can fix λ and, for brevity, we can omit it from notations in the course of this proof. For any $t > 0$ we have

$$\frac{L_{PED}(\hat{\beta}_1, \dots, \hat{\beta}_{j-1}, t, \hat{\beta}_{j+1}, \dots, \hat{\beta}_p) - L_{PED}(\hat{\beta}_1, \dots, \hat{\beta}_{j-1}, 0, \hat{\beta}_{j+1}, \dots, \hat{\beta}_p)}{t} \geq 0.$$

Again, for brevity we can denote $\hat{\beta}_{t@j} = (\hat{\beta}_1, \dots, \hat{\beta}_{j-1}, t, \hat{\beta}_{j+1}, \dots, \hat{\beta}_p)^T$ and also let $\hat{\theta}_{t@j}$ be the angle between $x_{*,j}$ and $Y - X\hat{\beta}_{t@j}$. By using the mean value theorem (Lagrange), there exists $0 < t^* < t$ such that

$$\frac{L_{PED}(\hat{\beta}_{t@j}) - L_{PED}(\hat{\beta}_{0@j})}{t} = -\cos(\hat{\theta}_{t^*@j}) + \lambda \frac{\sqrt{\|\hat{\beta}_{t@j}\| \cdot |\hat{\beta}_{t@j}|_1} - \sqrt{\|\hat{\beta}_{0@j}\| \cdot |\hat{\beta}_{0@j}|_1}}{t}$$

If we rationalize the numerator of the second fraction in the previous equation, we get

$$\frac{L_{PED}(\hat{\beta}_{t@j}) - L_{PED}(\hat{\beta}_{0@j})}{t} = -\cos(\hat{\theta}_{t^*@j}) + \lambda \frac{\frac{\|\hat{\beta}_{t@j}\| \cdot |\hat{\beta}_{t@j}|_1 - \|\hat{\beta}_{0@j}\| \cdot |\hat{\beta}_{0@j}|_1}{t}}{\sqrt{\|\hat{\beta}_{t@j}\| \cdot |\hat{\beta}_{t@j}|_1} + \sqrt{\|\hat{\beta}_{0@j}\| \cdot |\hat{\beta}_{0@j}|_1}}$$

and thus

$$\cos(\hat{\theta}_{t^*@j}) \leq \lambda \frac{\frac{\|\hat{\beta}_{t@j}\| \cdot |\hat{\beta}_{t@j}|_1 - \|\hat{\beta}_{0@j}\| \cdot |\hat{\beta}_{0@j}|_1}{t}}{\sqrt{\|\hat{\beta}_{t@j}\| \cdot |\hat{\beta}_{t@j}|_1} + \sqrt{\|\hat{\beta}_{0@j}\| \cdot |\hat{\beta}_{0@j}|_1}}.$$

Also

$$\frac{\|\hat{\beta}_{t@j}\| \cdot |\hat{\beta}_{t@j}|_1 - \|\hat{\beta}_{0@j}\| \cdot |\hat{\beta}_{0@j}|_1}{t} = |\hat{\beta}_{t@j}|_1 \frac{\|\hat{\beta}_{t@j}\| - \|\hat{\beta}_{0@j}\|}{t} + \|\hat{\beta}_{0@j}\| \frac{|\hat{\beta}_{t@j}|_1 - |\hat{\beta}_{0@j}|_1}{t}$$

and we notice that $\frac{|\hat{\beta}_{t@j}|_1 - |\hat{\beta}_{0@j}|_1}{t} = 1$ for any $t > 0$. Letting $t \rightarrow 0$ we obtain

$$\cos(\hat{\theta}_{0@j}) \leq \frac{\lambda}{2} \sqrt{\frac{\|\hat{\beta}_{0@j}\|}{|\hat{\beta}_{0@j}|_1}} = \frac{\lambda \hat{k}}{2}.$$

Analogously, by starting with $t < 0$, we can show that

$$\cos(\hat{\theta}_{0@j}) \geq -\frac{\lambda}{2} \sqrt{\frac{\|\hat{\beta}_{0@j}\|}{|\hat{\beta}_{0@j}|_1}} = \frac{\lambda \hat{k}}{2}.$$

□

Proof. (Proposition 2) By writing the necessary conditions for optimality in the case of problem (3) we have

$$\text{sgn}(X_j^T(Y - X\hat{\beta})) = \text{sgn}\left(\frac{\pi}{2} - \hat{\theta}_j\right)$$

and

$$\frac{\hat{\beta}_j(\lambda)}{\|\hat{\beta}(\lambda)\|} = \hat{k} \left(\frac{2X_j^T(Y - X\hat{\beta})}{\lambda\|Y - X\hat{\beta}\|} - \text{sgn}(\hat{\beta}_j(\lambda))\hat{k} \right)$$

if $\hat{\beta}_j(\lambda) \neq 0$. Since $\hat{k} > 0$ we have $\text{sgn}(\hat{\beta}_j) = \text{sgn}(X_j^T(Y - X\hat{\beta})) = \text{sgn}(\cos(\hat{\theta}_j))$. \square

Proof. (Lemma 3) The proof follows directly from (5) and (6). \square

Proof. (Proposition 3) If $\hat{\beta}(\lambda)$ is a solution of (3) we have $\cos(\hat{\theta}_j) \leq \frac{\lambda}{2} \left(\hat{k} + \frac{M}{\hat{k}} \right)$ and therefore $\cos(\hat{\theta}_j) \rightarrow 0$ when $\lambda \rightarrow 0$ since $M \leq 1$ and $p^{-1/4} \leq \hat{k} \leq 1$. \square

Proof. (Theorem 3) The proof follows a similar method to that of Theorem 1 in Belloni et al (2011). Given that $\hat{\beta}(\lambda)$ is a minimizer of the PED objective function for a given λ , we have

$$L(\hat{\beta}(\lambda)) - L(\beta^*) \leq \lambda\|\beta^*\|_1 - \lambda\|\hat{\beta}(\lambda)\|_{(1,2)} \leq \lambda\|\beta^*\|_1 - \frac{\lambda}{\sqrt[4]{p}}\|\hat{\beta}(\lambda)\|_1.$$

We obtain

$$L(\hat{\beta}(\lambda)) - L(\beta^*) \leq \frac{\lambda}{\sqrt[4]{p}}\|\beta^*\|_1 - \frac{\lambda}{\sqrt[4]{p}}\|\hat{\beta}(\lambda)\|_1 + \sqrt[4]{p}\lambda M^* \leq \frac{\lambda}{\sqrt[4]{p}}(\|\tilde{u}\|_1 - \|\tilde{u}^c\|_1) + \lambda M^* \sqrt[4]{p^*}.$$

At the same time, due to the convexity of L , we have

$$L(\hat{\beta}(\lambda)) - L(\beta^*) \geq (\nabla L(\beta^*))^T u \geq -\frac{\|X^T \epsilon\|_\infty}{\|\epsilon\|} \|u\|_1 \geq -\frac{\lambda}{c\sqrt[4]{p}}(\|\tilde{u}\|_1 + \|\tilde{u}^c\|_1)$$

if $\lambda \geq c\sqrt[4]{p}S$, where $S = \frac{\|X^T \epsilon\|_\infty}{\|\epsilon\|}$. Thus we have

$$\|\tilde{u}^c\|_1 \leq \frac{c+1}{c-1}\|\tilde{u}\|_1 + \frac{c\sqrt[4]{p}}{c-1}\sqrt[4]{p^*}M^*$$

and also

$$\|u\|_1 \leq \frac{2c}{c-1}\|\tilde{u}\|_1 + \frac{c\sqrt[4]{p}}{c-1}\sqrt[4]{p^*}M^*.$$

Now

$$\begin{aligned} L(\hat{\beta}(\lambda)) - L(\beta^*) &\leq |L(\hat{\beta}(\lambda)) - L(\beta^*)| \leq \frac{\lambda}{c\sqrt[4]{p}}(\|\tilde{u}\|_1 + \|\tilde{u}^c\|_1) \\ &\leq \frac{\lambda\|\tilde{u}\|_1}{c\sqrt[4]{p}} \leq \frac{\lambda\sqrt{p^*}\|u\|_X}{\sqrt[4]{p}k_c^*}. \end{aligned}$$

Considering the identity

$$L^2(\hat{\beta}(\lambda)) - L^2(\beta^*) = \|u\|_X^2 - 2(\sigma\epsilon^T Xu)$$

along with

$$L^2(\hat{\beta}(\lambda)) - L^2(\beta^*) = (L(\hat{\beta}(\lambda)) - L(\beta^*))(L(\hat{\beta}(\lambda)) + L(\beta^*))$$

and the fact that

$$2|\sigma\epsilon^T Xu| \leq 2L(\beta^*)S\|u\|_1$$

we deduce

$$\begin{aligned} \|u\|_X^2 &\leq \frac{\lambda\sqrt{p^*}\|u\|_X}{c\sqrt[4]{p}k_c^*} \left(L(\beta^*) + \frac{\lambda\sqrt{p^*}\|u\|_X}{\sqrt[4]{p}k_c^*} \right) + L(\beta^*) \frac{\lambda\sqrt{p^*}\|u\|_X}{\sqrt[4]{p}k_c^*}, \\ &\leq \frac{2\lambda\sqrt{p^*}\|u\|_X}{\sqrt[4]{p}k_c^*} + \left(\frac{\lambda\sqrt{p^*}\|u\|_X}{\sqrt[4]{p}k_c^*} \right)^2. \end{aligned}$$

Thus we have

$$\left[1 - \left(\frac{\lambda\sqrt{p^*}}{\sqrt[4]{p}k_c^*} \right)^2 \right] \|u\|_X^2 \leq \frac{2\lambda\sqrt{p^*}}{\sqrt[4]{p}k_c^*} L(\beta^*) \|u\|_X.$$

We write $\lambda \leq \frac{\rho\sqrt{p^*}}{\sqrt[4]{p}k_c^*}$ where $0 < \rho < 1$ and $\lambda = \frac{c\sqrt[4]{p}}{\sqrt{n}}\Phi_0^{-1}\left(1 - \frac{\alpha}{2p}\right)$, and we can use the result that $\Phi_0^{-1}\left(1 - \frac{\alpha}{2p}\right) \leq \sqrt{2\log(2p/\alpha)}$ (from Belloni et al., 2011). Hence,

$$(1 - \rho^2)\|u\|_X \leq \frac{2c\sqrt{p^*}\sqrt{\log(2p/\alpha)}L(\beta^*)}{k_c^*\sqrt{n}},$$

and so

$$\bar{k}_c^*\|\hat{\beta}(\lambda) - \beta^*\| \leq \frac{\text{const.}\sqrt{p^*\log(2p/\alpha)}L(\beta^*)}{(1 - \rho^2)n}.$$

Proof. (Corollary 1) We have

$$\begin{aligned} L(\hat{\beta}(\lambda)) - L(\beta^*) &\leq \frac{\lambda\sqrt{n}}{\sqrt[4]{p}}\|\beta^*\|_1 - \frac{\lambda\sqrt{n}}{\sqrt[4]{p}}\|\hat{\beta}(\lambda)\|_1 + \lambda \left(\frac{\sqrt{n}}{\sqrt[4]{p}}\|\hat{\beta}(\lambda)\|_1 - \|\hat{\beta}(\lambda)\|_{(1,2)} \right) + \\ &\quad \lambda\|\beta^*\|_1 \left(1 - \frac{\sqrt{n}}{\sqrt[4]{p}} \right). \end{aligned}$$

If $\frac{\lambda\sqrt{n}}{c\sqrt[4]{p}} \geq S$ with probability $1 - \alpha$ for some $c > 1$, we obtain

$$\begin{aligned} (19) \quad -\frac{\sqrt{n}}{c\sqrt[4]{p}}(\|\tilde{u}\|_1 + \|\tilde{u}^c\|_1) &\leq \frac{\sqrt{n}}{\sqrt[4]{p}}\|\tilde{u}\|_1 - \frac{\sqrt{n}}{\sqrt[4]{p}}\|\tilde{u}^c\|_1 + \left(\frac{\sqrt{n}}{\sqrt[4]{p}}\|\hat{\beta}(\lambda)\|_1 - \|\hat{\beta}(\lambda)\|_{(1,2)} \right) + \\ &\quad \|\beta^*\|_1 \left(1 - \frac{\sqrt{n}}{\sqrt[4]{p}} \right). \end{aligned}$$

At the same time we can write

$$\begin{aligned} \left(\frac{\sqrt{n}}{\sqrt[4]{p}}\|\hat{\beta}(\lambda)\|_1 - \|\hat{\beta}(\lambda)\|_{(1,2)} \right) + \|\beta^*\|_1 \left(1 - \frac{\sqrt{n}}{\sqrt[4]{p}} \right) &= \|\hat{\beta}(\lambda)\|_1 \left(\frac{\sqrt{n}}{\sqrt[4]{p}} - \sqrt{\frac{\|\hat{\beta}(\lambda)\|}{\|\hat{\beta}(\lambda)\|_1}} \right) + \\ &\quad \|\beta^*\|_1 \left(\sqrt{\frac{\|\hat{\beta}(\lambda)\|}{\|\hat{\beta}(\lambda)\|_1}} - \frac{\sqrt{n}}{\sqrt[4]{p}} \right) + \|\beta^*\|_1 \left(1 - \frac{\sqrt{n}}{\sqrt[4]{p}} \right) \end{aligned}$$

and thus we have

$$\left(\frac{\sqrt{n}}{\sqrt[4]{p}}\|\hat{\beta}(\lambda)\|_1 - \|\hat{\beta}(\lambda)\|_{(1,2)}\right) + \|\beta^*\|_1 \left(1 - \frac{\sqrt{n}}{\sqrt[4]{p}}\right) \leq \|u\|_1 \left(\frac{\sqrt{n}}{\sqrt[4]{p}} - \sqrt{\frac{\|\hat{\beta}(\lambda)\|}{\|\hat{\beta}(\lambda)\|_1}}\right) + \|\beta^*\|_1 \left(1 - \frac{\sqrt{n}}{\sqrt[4]{p}}\right).$$

By combining with inequality (19) we obtain

$$\frac{\sqrt{n}}{\sqrt[4]{p}} \left(1 - \frac{1}{c}\right) \|\tilde{u}^c\|_1 \leq \frac{\sqrt{n}}{\sqrt[4]{p}} \|\tilde{u}\|_1 \left(1 + \frac{1}{c}\right) + \|u\|_1 \left(\frac{\sqrt{n}}{\sqrt[4]{p}} - \sqrt{\frac{\|\hat{\beta}(\lambda)\|}{\|\hat{\beta}(\lambda)\|_1}}\right) + \|\beta^*\|_1 \left(1 - \frac{\sqrt{n}}{\sqrt[4]{p}}\right)$$

and it immediately follows that

$$\|u\|_1 \left(\sqrt{\frac{\|\hat{\beta}(\lambda)\|}{\|\hat{\beta}(\lambda)\|_1}} - \frac{\sqrt{n}}{c\sqrt[4]{p}}\right) \leq \frac{2\sqrt{n}}{\sqrt[4]{p}} \|\tilde{u}\|_1 + \|\beta^*\|_1 \left(1 - \frac{\sqrt{n}}{\sqrt[4]{p}}\right).$$

If $\sqrt{\frac{\|\hat{\beta}(\lambda)\|}{\|\hat{\beta}(\lambda)\|_1}} - \frac{\sqrt{n}}{c\sqrt[4]{p}} \geq \xi > 0$ we have

$$\|u\|_1 \leq \frac{2\sqrt{n}}{\xi\sqrt[4]{p}} \|\tilde{u}\|_1 + \frac{\|\beta^*\|_1}{\xi} \left(1 - \frac{\sqrt{n}}{\sqrt[4]{p}}\right).$$

and equivalently

$$\|\tilde{u}^c\|_1 \xi \leq \|\tilde{u}\|_1 \left(\frac{2\sqrt{n}}{\sqrt[4]{p}} - \xi\right) + \|\beta^*\|_1 \left(1 - \frac{\sqrt{n}}{\sqrt[4]{p}}\right).$$

Considering $\Delta_\xi = \left\{u \in \mathbb{R}^p, \|\tilde{u}^c\|_1 \xi \leq \|\tilde{u}\|_1 \left(\frac{2\sqrt{n}}{\sqrt[4]{p}} - \xi\right) + \|\beta^*\|_1 \left(1 - \frac{\sqrt{n}}{\sqrt[4]{p}}\right)\right\}$ and assuming

$$k_\xi^* = \min_{u \in \Delta_\xi} \frac{\frac{\sqrt{p^*}}{\sqrt{n}} \|u\|_X}{\frac{2\sqrt{n}}{\xi\sqrt[4]{p}} \|\tilde{u}\|_1 + \frac{\|\beta^*\|_1}{\xi} \left(1 - \frac{\sqrt{n}}{\sqrt[4]{p}}\right)} > k > 0$$

we get

$$\begin{aligned} L(\hat{\beta}(\lambda)) - L(\beta^*) &\leq |L(\hat{\beta}(\lambda)) - L(\beta^*)| \leq \frac{\lambda\sqrt{n}}{c\sqrt[4]{p}} (\|\tilde{u}\|_1 + \|\tilde{u}^c\|_1) \\ &\leq \frac{\lambda\sqrt{n}\|u\|_1}{c\sqrt[4]{p}} \leq \frac{\lambda\sqrt{p^*}\|u\|_X}{\sqrt[4]{p}k_\xi^*}. \end{aligned}$$

The rest of the proof is virtually identical with the last part of the argument we detailed for Theorem 3.

□

DEPARTMENT OF MATHEMATICS, COLLEGE OF WILLIAM & MARY, WILLIAMSBURG, VIRGINIA, 23185, USA

E-mail address: dvasiliu@wm.edu

DEPARTMENT OF QUANTITATIVE HEALTH SCIENCES, LERNER RESEARCH INSTITUTE, CLEVELAND CLINIC, CLEVELAND, OHIO, 44195, USA

E-mail address: deyt@ccf.org

SCHOOL OF MATHEMATICAL SCIENCES, THE UNIVERSITY OF NOTTINGHAM, NOTTINGHAM, NG7 2RD, UK

E-mail address: ian.dryden@nottingham.ac.uk